Momentum spectrometry of spherical harmonics and a probe of geometric embedding effect

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As a submanifold is embedded into higher dimensional flat space, quantum mechanics gives various embedding quantities, e.g., the geometric momentum and geometric potential, etc. For a particle moving on a two-dimensional sphere or a free rotation of a spherical top, the projections of the geometric momentum $\mathbf{p}$ and the angular momentum $\mathbf{L}$ onto a certain Cartesian axis form a complete set of commuting observables as $[p_i, L_i] = 0$ $(i = 1, 2, 3)$. We have therefore a (p_i, L_i) representation for the states on the two-dimensional spherical surface. The geometric momentum distribution of the ground states for a freely rotating rigid rotor seems within the resolution power of present momentum spectrometer and can be measured to probe the embedding effect.

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I. INTRODUCTION

In microscopic domain, there are many quantum motions confined on the two-dimensional surfaces, e.g., mobile carriers on the corrugating graphene sheet or spherical fullerene molecule C_{60}, and free rotation of hydrogen nuclei around its center of mass in a hydrogen molecule at relatively low temperature, etc. Over the past decade, we have witnessed that physics community gradually reaches consensus that the examination of the quantum motions confined on the two-dimensional surfaces in three-dimensional Euclidean space R^3 is of physical significance. In the Euclidean space, the quantum physics is well defined, one can use conventional quantum mechanics without any new postulate imposed [1, 2]. The confinement of the particle on a curved two-dimensional manifold is physically treated as the limiting case of a particle in a three-dimensional manifold that has a confining potential acting in the normal direction of its two-dimensional surface, and we can then have an unambiguous formulation of quantum mechanics on the surface as a secondary or derived theory [3–19]. However, if we hope to give the same theory within the Dirac's theory for a systems with second class constraints [2], some cautions need to be taken into consideration [20]. We can then have an effective formulation of quantum mechanics on the surface as a secondary or derived theory. When no electromagnetic field is applied and the spin of the particle plays insignificant role, the marked feature of the theory is the dependence of both an effective potential V_g [21] in the Hamiltonian and the geometric momentum $\mathbf{p}$ on the mean curvature M [3, 4, 9–13]. In simple and plain words, the mean curvature M, on one hand, is an extrinsic curvature that is not detectable to someone who can not study the three-dimensional space surrounding the surface on which he resides, whereas the gaussian curvature K, on the other hand, is an intrinsic curvature that is detectable to the "two-dimensional inhabitants" on a surface and not just outside observers [22]. So, in purely intrinsic geometry, undefinable and even meaningless is the shape itself of a surface.

The geometric potential [3, 4, 21] with μ denoting the mass ,

$$V_g = -\hbar^2/(2\mu)(M^2 - K) \tag{1}$$

comes from how to define a proper form of Laplacian operator acting on a quantum state on surface [12, 13, 23, 24], whereas the geometric momentum with ∇_2 being the gradient operator on a two-dimensional surface [25] and $\mathbf{n}$ standing for the normal vector of the surface,

$$\mathbf{p} = -i\hbar(\nabla_2 + M\mathbf{n}), \tag{2}$$

is related to a proper form of gradient operator on the state [12, 13]. One can also call them embedding potential [26] and embedding momentum, respectively. So, they have not only the common geometric origin but can be all derived from the same physical treatment [13]. An experimental verification of the potential amounts to an indirect affirmative experimental evidence of the momentum as well, and *vice versa*. The geometric potential has recently been experimentally verified [18, 19], and it is an important advance in quantum mechanics, implying that quantum mechanics based on purely intrinsic geometry does not offer a proper description of the constrained motions in microscopic domain, provided that the extrinsic curvature must be included as well. Here we mention that the spin

of the particle usually plays a role via the surface spin-orbit coupling [14–16], etc.[17] obtained also from the same procedure of squeezed limit of its the three-dimensional analogue.

Finding out a novel suggestion that can be experimentally investigated is a decisive issue for further exploration of the various embedding effects. Noting that the linear momentum distribution of an electron state within a hydrogen atom can be easily carried out and had been experimentally verified [27, 28]. Let us consider the simplest constrained motion on two dimensional surface S^2. We may ask if it is possible to give a momentum space representation for the states on S^2? An immediate problem is what the proper momentum is. It can never be the usual linear momentum $-i\hbar\nabla = -i\hbar(\partial_x, \partial_y, \partial_z)$ because the motion on S^2 has only two degrees of freedom while $-i\hbar\nabla$ has three independent components that are too many to form a complete set of commuting observables for S^2. Moreover, as we stress before [12], a set of self-adjoint momentum operators in purely intrinsic geometry is unattainable for any states on S^2, and the geometric momentum $\mathbf{p} = -i\hbar(\nabla_2 + M\mathbf{n})$ (2) alone does not suffice because its three components are not mutually commutable, thus too few to provide a complete set of commuting observables.

The present paper first starts from a dynamical symmetric group $SO(3.1)$ on the sphere to give a proper a complete set of commuting observables, to arrive at a dynamical representation mixing the geometric momentum and orbital angular momentum. Second, it aims at an experimental proposal to probe the fundamental embedding effect via the measurement of the geometric momentum distribution of the some molecular rotational states.

II. GEOMETRIC MOMENTUM – ANGULAR MOMENTUM REPRESENTATION ON S^2

The three Cartesian components of the geometric momentum $\mathbf{p}$ on the two-dimensional spherical surface of fixed radius r are from (2) with $M = -1/r$ [12, 13, 23, 29–31],

$$p_x = -i\hbar(\cos\theta\cos\varphi\frac{\partial}{\partial\theta} - \frac{\sin\varphi}{\sin\theta}\frac{\partial}{\partial\varphi} - \sin\theta\cos\varphi), \tag{3}$$

$$p_y = -i\hbar(\cos\theta\sin\varphi\frac{\partial}{\partial\theta} + \frac{\cos\varphi}{\sin\theta}\frac{\partial}{\partial\varphi} - \sin\theta\sin\varphi), \tag{4}$$

$$p_z = i\hbar(\sin\theta\frac{\partial}{\partial\theta} + \cos\theta), \tag{5}$$

where the transformation $p_i r \to p_i$ is made to conveniently convert the momentum into dimension of the angular momentum, i.e., the dimension of Planck's constant $\hbar$. The three Cartesian components of the orbital angular momentum $\mathbf{L}$ are well-known as $L_x = i\hbar(\sin\varphi\partial_\theta + \cot\theta\cos\varphi\partial_\varphi)$, $L_y = -i\hbar(\sin\varphi\partial_\theta - \cot\theta\sin\varphi\partial_\varphi)$ and $L_z = -i\hbar\partial_\varphi$.

We can easily verify the following commutation relations that form an $so(3.1)$ algebra [12]:

$$[p_i, p_j] = -i\hbar\varepsilon_{ijk}L_k,\ [L_i, p_j] = i\hbar\varepsilon_{ijk}p_k,\ [L_i, L_j] = i\hbar\varepsilon_{ijk}L_k, \tag{6}$$

and

$$[L_i, p_i] = 0,\ (i = 1, 2, 3). \tag{7}$$

We see that the quantum motion on the sphere of geometric $O(3)$ symmetry possesses a dynamical $SO(3.1)$ symmetry. Three commutable pairs (L_i, p_i) are equivalent with each other upon a rotation of coordinate system [12, 32],

$$f_x = \exp(-i\pi L_y/2) f_z \exp(i\pi L_y/2),\ \ f_y = \exp(i\pi L_x/2) f_z \exp(-i\pi L_x/2),\ \ (f_i \to L_i \text{ or } p_i). \tag{8}$$

Here we follow the convention that a rotation operation affects a physical system itself [33]. Equation (8) above implies that it is sufficient to study one representation determined by one pair of the three (L_i, p_i).

Because motion on S^2 has two degrees of freedom, a representation needs a complete set of a complete set of two commuting observables. The well-known set is the spherical harmonics $Y_{lm}(\theta, \varphi)$ determined by the commutable pairs (L^2, L_z) in the (θ, φ) representation. For convenience of a comparison between basis vectors $Y_{lm}(\theta, \varphi)$ and new ones span by a complete set of simultaneous functions given by both the geometric and the angular momentum, we choose the z-axis component pair (p_z, L_z) rather than (p_x, L_x) or (p_y, L_y). The common operator L_z means also a choice of the reference direction in position space.

The complete set of the simultaneous eigenfunctions for (p_z, L_z) is given by,

$$\psi_{p_z,m}(\theta, \varphi) = \frac{1}{\sqrt{2\pi\hbar}}\frac{1}{\sin\theta}\tan^{-\frac{ip_z}{\hbar}}\left(\frac{\theta}{2}\right)\frac{1}{\sqrt{2\pi}}e^{im\varphi}. \tag{9}$$

The eigenvalues of (p_z, L_z) acting on $\psi_{p_z,m}(\theta,\varphi)$ above are $(p_z, m\hbar)$ respectively. The normalization relation can be easily verified,

$$\begin{aligned}
&\oint \psi^*_{p'_z m'}(\theta,\phi)\,\psi_{p_z,m}(\theta,\varphi)\sin\theta d\theta d\varphi \\
&= \delta_{m'm}\frac{1}{2\pi\hbar}\int_0^\pi \exp\left(i\frac{(p'_z - p_z)}{\hbar}(\ln\tan\frac{\theta}{2})\right)\frac{1}{\sin\theta}d\theta \\
&= \delta_{m'm}\frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} \exp\left(i\frac{(p'_z - p_z)}{\hbar}u\right)du \\
&= \delta_{m'm}\delta\left(p'_z - p_z\right), \qquad (10)
\end{aligned}$$

where the variable transformation

$$\ln\tan\theta/2 \to u, \text{ or } \theta \to 2\arctan(e^u), (u \in (-\infty,\infty)), \tag{11}$$

is used, and $\delta_{m'm}$ is the Kronecker delta that equals to 1 once $m' = m$ and to zero otherwise. This variable transformation (11) has the following profound consequence: It makes the operator p_z (5) behave like a linear momentum which is defined on flat space $u \in (-\infty,\infty)$,

$$p_z(\theta) \longrightarrow p_z(u) = i\hbar\frac{\partial}{\partial u}, \tag{12}$$

whose eigenfunction is well-known as $exp(-iup_z/\hbar)/\sqrt{2\pi\hbar}$ corresponding to eigenvalue p_z.

To give the (p_z, L_z) representation of the operators and states, we for convenience utilize the same variable transformation (11) and will use u instead of θ in all relevant states and operators. For square of the angular momentum operator,

$$L^2(\theta,\varphi) = -\hbar^2(\frac{\partial^2}{\partial\theta^2} + \cot\theta\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}), \tag{13}$$

we have,

$$L^2(\theta,\varphi) \to L^2(u,\varphi) = -\hbar^2\cosh^2(u)\left(\frac{\partial^2}{\partial u^2} + 2\tanh(u)\frac{\partial}{\partial u} + \frac{\partial^2}{\partial\varphi^2} + 1\right). \tag{14}$$

For spherical harmonics $Y_{lm}(u,\varphi)$ (that can also be directly obtained by solving the eigenvalue equation $L^2(u,\varphi)Y_{lm}(u,\varphi) = \lambda Y_{lm}(u,\varphi)$), we have

$$Y_{lm}(\theta,\varphi) \to Y_{lm}(u,\varphi) = N_{lm}\frac{P_l^m(-\tanh u)}{\cosh u}\frac{1}{\sqrt{2\pi}}e^{im\varphi}, \tag{15}$$

where,

$$N_{lm} = \sqrt{\frac{2l+1}{2}\frac{(l-1)!}{(l+m)!}}.$$

The normalization of the spherical harmonics $Y_{lm}(u,\varphi)$ satisfies,

$$\delta_{l'l}\delta_{m'm} = \oint Y^*_{l'm'}(\theta,\varphi)Y_{lm}(\theta,\varphi)\sin\theta d\theta d\varphi = \int_0^{2\pi}\left[\int_{-\infty}^{\infty} Y_{l'm'}(u,\varphi)Y_{lm}(u,\varphi)du\right]d\varphi. \tag{16}$$

It implies that the transformed system is defined on two dimensional stripe space: $u \in (-\infty,\infty) \cup \varphi \in (0, 2\pi)$.

A wave function $\Phi(p_z, L_z)$ in (p_z, L_z) representation corresponding to the position wave function $\Psi(u,\varphi)$ is in general,

$$\Phi(p_z, L_z) = \int_0^{2\pi}\left[\int_{-\infty}^{\infty}\Psi(u,\varphi)\frac{\exp\left(i\frac{p_z}{\hbar}u\right)}{\sqrt{2\pi\hbar}}du\right]\frac{e^{-im\varphi}}{\sqrt{2\pi}}d\varphi. \tag{17}$$

For u- dependent part of the spherical harmonics $Y_{lm}(u,\varphi)$ we get from (15),

$$\begin{aligned} Q_{lm}(p_z) &= N_{lm}\int_{-\infty}^{\infty}\frac{P_l^m(-\tanh u)}{\cosh u}\frac{1}{\sqrt{2\pi\hbar}}\exp\left(i\frac{p_z}{\hbar}u\right)du, \\ &= N_{lm}F(p_z,\left[\frac{P_l^m(-\tanh u)}{\cosh u}\right]), \end{aligned} \tag{18}$$

where the Fourier transform $F(p,[f(q)])$ of a function $f(q)$ is defined by,

$$F(p,[f(q)]) \equiv \int f(q)\frac{e^{ipq}}{\sqrt{2\pi}}dq. \tag{19}$$

For φ- dependent part of the spherical harmonics $Y_{lm}(u,\varphi)$ we get in the (p_z, L_z) representation a simple Kronecker delta function $\delta_{L_z,m\hbar}$. So the spherical harmonics $Y_{lm}(p_z,L_z)$ becomes,

$$Y_{lm}(u,\varphi)\to Y_{lm}(p_z,L_z) = N_{lm}F(p_z,\left[\frac{P_l^m(-\tanh u)}{\cosh u}\right])\delta_{L_z,m\hbar}. \tag{20}$$

The acting of an operator on the wave function $\Psi(u,\varphi)$ as $F(u,\varphi)\Psi(u,\varphi)$ in the (p_z,L_z) representation is given by from (17)

$$\begin{aligned} F(u,\varphi)\Psi(u,\varphi) &\to \int_0^{2\pi}\left[\int_{-\infty}^{\infty}(F(u,\varphi)\Psi(u,\varphi))\frac{\exp\left(i\frac{p_z}{\hbar}u\right)}{\sqrt{2\pi\hbar}}du\right]\frac{e^{-im\varphi}}{\sqrt{2\pi}}d\varphi \\ &= \int_0^{2\pi}\left[\int_{-\infty}^{\infty}(F(-i\hbar\frac{\partial}{\partial p_z},\varphi)\frac{\exp\left(i\frac{p_z}{\hbar}u\right)}{\sqrt{2\pi\hbar}}\Psi(u,\varphi))du\right]\frac{e^{-im\varphi}}{\sqrt{2\pi}}d\varphi \\ &= F(-i\hbar\frac{\partial}{\partial p_z},L_z)\Phi(p_z,L_z). \end{aligned} \tag{21}$$

Applying above results (17), (18) and (21) to both sides of the eigenvalue function $L^2(u,\varphi)Y_{lm}(u,\varphi) = l(l+1)\hbar^2 Y_{lm}(u,\varphi)$, we have,

$$L^2(u,\varphi)Y_{lm}(u,\varphi) = l(l+1)\hbar^2 Y_{lm}(u,\varphi) \to L^2(p_z,L_z)Q_{lm}(p_z)\delta_{L_z,m\hbar} = l(l+1)\hbar^2 Q_{lm}(p_z)\delta_{L_z,m\hbar}, \tag{22}$$

where the essential part is the equation for $Q_{lm}(p_z)$,

$$\begin{aligned} &N_{lm}\int_0^{2\pi}\left[\left(p_z^2+2i\hbar p_z\tanh(u)+(m^2-1)\hbar^2\right)\cosh^2(u)\frac{\exp\left(i\frac{p_z}{\hbar}u\right)}{\sqrt{2\pi\hbar}}\frac{P_l^m(-\tanh u)}{\cosh u}du\right] \\ &= l(l+1)\hbar^2 Q_{lm}(p_z). \end{aligned} \tag{23}$$

This equation (23) in fact has following two equivalent forms. One is a differential equation from (21)

$$\left(p_z^2+2i\hbar p_z\tanh(-i\hbar\frac{\partial}{\partial p_z})+(m^2-1)\hbar^2\right)\cosh^2(-i\hbar\frac{\partial}{\partial p_z})Q_{lm}(p_z) = l(l+1)\hbar^2 Q_{lm}(p_z). \tag{24}$$

Another is a difference equation with use of a relation: $\exp(\pm au)\exp(ip_z u/\hbar) = \exp(ip_z(u\mp ia\hbar)/\hbar)$,

$$\begin{aligned} l(l+1)\hbar^2 Q_{lm}(p_z) &= \frac{1}{2}\left[p_z^2+(m^2-1)\hbar^2\right]Q_{lm}(p_z) \\ &+\frac{1}{4}\left[p_z^2+(m^2-1)\hbar^2+2i\hbar p_z\right]Q_{lm}(p_z-i2\hbar) \\ &+\frac{1}{4}\left[p_z^2+(m^2-1)\hbar^2-2i\hbar p_z\right]Q_{lm}(p_z+i2\hbar), \end{aligned} \tag{25}$$

The similar difference equation appears in many systems, e.g. Morse oscillator in momentum space [34]. The following properties of $Q_{lm}(p_z)$ are available. 1, Orthogonality from Eq.(16):

$$\int_{-\infty}^{\infty}Q_{l'm'}^*(p_z)Q_{lm}(p_z)dp_z = \delta_{l'l}\delta_{m'm}. \tag{26}$$

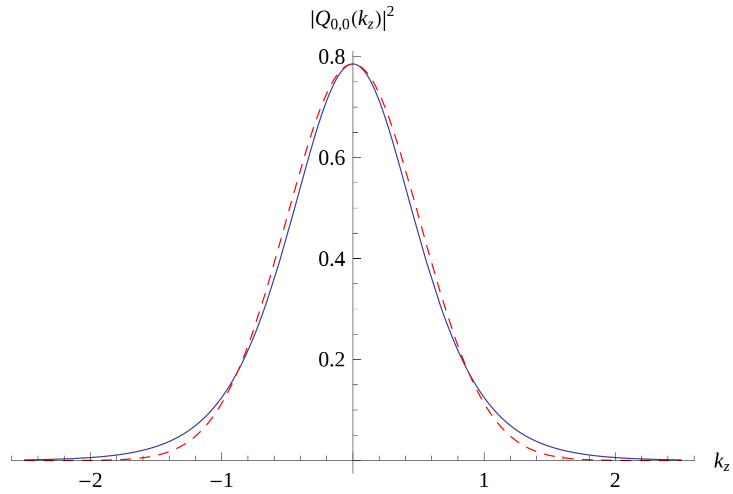

FIG. 1: Geometric momentum distribution density for the ground state of ground rotational state $Y_{0,0} = 1/(\sqrt{4\pi})$ (solid line), and the momentum distribution density for the ground state of one-dimensional simple harmonic oscillator (dashed line). They are almost identical. In all figures, the dimensionless momentum $k_z \equiv p_z/\hbar$ is used.

2, Symmetries from Eq.(18):

$$Q_{l(-m)}(p_z) = (-1)^m Q_{lm}(p_z), Q_{lm}(-p_z) = (-1)^m Q_{lm}(p_z). \tag{27}$$

3, It can be verified that for a given quantum number l, they are $l+1$ linearly independent lth polynomials upon factors of $\text{sech}(\pi p_z/(2\hbar))$ corresponding to $m = 0, 2, 4, ...$ or $\text{csch}(\pi p_z/(2\hbar))$ corresponding to odd m.

Thus, a dynamical (p_z, L_z) representation on S^2 is established.

III. MOMENTUM SPECTROMETER FOR SOME ROTATIONAL STATES

We now use the dynamical representation to give the momentum distribution of some rotational states, and then suggest a search for the embedding effect via the measurement of the distribution.

The first nine state functions of $Q_{lm}(p_z)$ for $l = 0$, $l = 1$, and $l = 2$ are from (18),

$$Q_{0,0}(p_z) = \frac{1}{2}\sqrt{\pi}\text{sech}\left(\frac{\pi}{2}\frac{p_z}{\hbar}\right) \tag{28}$$

$$Q_{1,0}(p_z) = -\frac{1}{2}i\sqrt{3\pi}\frac{p_z}{\hbar}\text{sech}\left(\frac{\pi}{2}\frac{p_z}{\hbar}\right),\; Q_{1,\pm1}(p_z) = \pm\frac{1}{2}\sqrt{\frac{3\pi}{2}}\frac{p_z}{\hbar}\text{csch}\left(\frac{\pi}{2}\frac{p_z}{\hbar}\right), \tag{29}$$

$$Q_{2,0}(p_z) = -\frac{1}{8}\sqrt{5\pi}\left(3(\frac{p_z}{\hbar})^2 - 1\right)\text{sech}\left(\frac{\pi}{2}\frac{p_z}{\hbar}\right),\; Q_{2,\pm1}(p_z) = \pm\frac{1}{4}i\sqrt{\frac{15\pi}{2}}(\frac{p_z}{\hbar})^2\text{csch}\left(\frac{\pi}{2}\frac{p_z}{\hbar}\right), \tag{30}$$

$$Q_{2,\pm2}(p_z) = \frac{1}{8}\sqrt{\frac{15\pi}{2}}\left((\frac{p_z}{\hbar})^2 + 1\right)\text{sech}\left(\frac{\pi}{2}\frac{p_z}{\hbar}\right). \tag{31}$$

For cases $l = 0$, $l = 3$, and $l = 10$, the probability distributions $|Q_{lm}(p_z)|^2$ of the dimensionless geometric momentum $k_z \equiv p_z/\hbar$ for rotational states represented by spherical harmonics $Y_{lm}(\theta, \varphi)$ are plotted in Figures 1, 2, and 3 respectively. In overall, they bear striking resemblance to the probability amplitude of the dimensionless momentum for one-dimensional simple harmonic oscillator. It is perfectly understandable that from the force operator $\dot{p}_i \equiv [p_i, H]/(i\hbar) = -\{x_i/r, H\} \sim -x_i$ with $\{U, V\} \equiv UV + VU$, we see that for the stationary state, the force is restoring and proportional to the displacement.

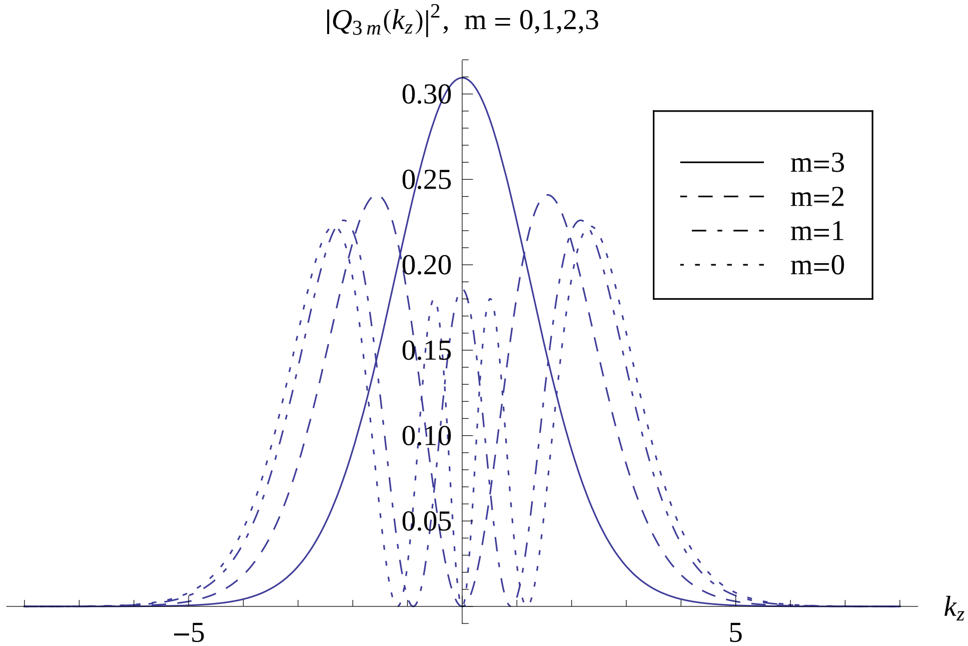

FIG. 2: Geometric momentum distribution density for the rotational states $Y_{lm}(\theta, \varphi)$ with $l = 1$ and $m = 0, 1, 2, 3$, they have number of nodes $3, 2, 1, 0$ respectively.

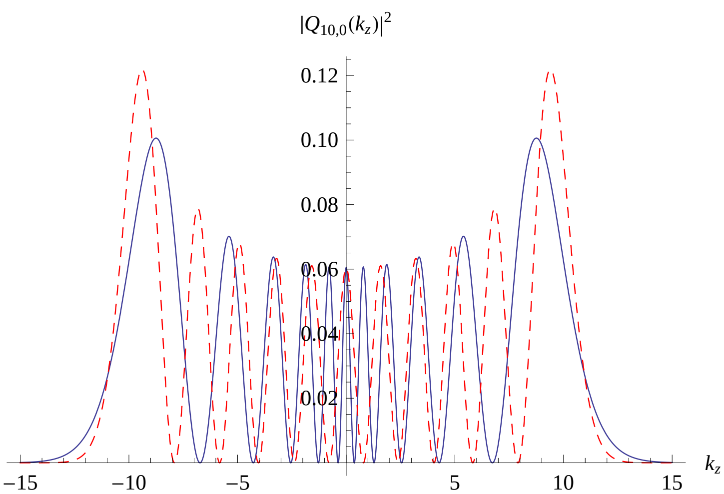

FIG. 3: Geometric momentum distribution density for rotational state $Y_{10,0}(\theta, \varphi)$ (solid line), and the momentum distribution density for the 10th excited state of one-dimensional simple harmonic oscillator (dashed line). Since both probabilities in a small interval Δk_z are almost the same, they have the same classical limit: the simple harmonic oscillation.

The rotation of a homonuclear diatomic molecule around its center of mass, and the free rotation of spherical cage molecule C_{60} or Au_{32} [35] around its center, etc.[36], can be well modelled by a spherical top. The ground state $Y_{00}(\theta, \varphi) = 1/\sqrt{4\pi}$ is the minimum uncertainty state for three pairs of (x_i, p_i) and $\Delta x_i \Delta p_i = \hbar/3$ (hereafter we restore p_i without multiplying the radius r as doing in (3)-(5)). The state $Y_{00}(\theta, \varphi)$ bears neither energy nor angular momentum, and the presence of zero-point the momentum fluctuation $\Delta p_i = \hbar/(\sqrt{3}r)$ contradicts what classical mechanics would indicate. With preparing these molecules into ground state of rotation, the probability density of the geometric momentum distribution is given by $|Q_{0,0}(p_z)|^2$ (28). With $r \approx 5.0$Å for C_{60}, $\Delta p_i \approx 0.07 a.u.(1 a.u. = \hbar/a_0$, with a_0 denoting the Bohr radius) and $r \approx 1.0$Å for H_2, $\Delta p_i \approx 0.3 a.u.$ that seems within the resolution power of a recently designed momentum spectrometer [37–39]. Moreover, if it is possible to prepare these molecules into any excited states, the momentum distributions $|Q_{lm}(p_z)|^2$ are given by Eq. (18).

IV. CONCLUSIONS AND DISCUSSIONS

How to understand quantum motions on a surface had been considered out of the problem. This might be due to the fact that in elementary particle physics and quantum gravity, physicists were acquainted with a fact that the outer space of the universe had little effect on the inner space [26]. Thus, consideration of the extrinsic curvature of two-dimensional surfaces was thought sheer nonsense, and the intrinsic property of the surfaces suffices in physics, which does not depend on whether they are embedded into the three-dimensional Euclidean, even higher-dimensional, space or not [26].

For motions on two dimensional spherical surface S^2, there is a new dynamical symmetry obeying $SO(3.1)$ group whose six generators are the Cartesian components of the geometric momentum $\mathbf{p}$ and the orbital angular momentum $\mathbf{L}$, where the dependence of the geometric momentum on extrinsic curvature, the mean curvature, reflects an embedding effect. From the commutation relations $[L_i, p_i] = 0$, $(i = 1, 2, 3)$, we have three complete sets of commuting observables, and they are equivalent with each other upon a rotation of coordinates. Thus a novel dynamical representation based on two observables, (p_z, L_z) in the present paper, is successfully constructed, and any states on S^2 can go through a momentum analysis.

Because the free rotation is ubiquitous in microscopic domain, we propose to measure the momentum distribution of the ground state of spherical harmonics to probe the embedding effect, once preparing the some molecules into the state. This kind of experiments seems within reach of the present nanotechnological capabilities [37–43].

Acknowledgments

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[1] P. A. M. Dirac, *The Principles of Quantum Mechanics*, 4th ed. (Oxford University Press, Oxford, 1967).
[2] P. A. M. Dirac, *Lectures on quantum mechanics* (Yeshiva University, New York, 1964); Can. J. Math. **2**, 129(1950).
[3] H. Jensen and H. Koppe, Ann. Phys. **63**, 586(1971).
[4] R. C. T. da Costa, Phys. Rev. A **23**, 1982(1981).
[5] M. Ikegami and Y. Nagaoka, S. Takagi and T. Tanzawa, Prog. Theoret. Phys. **88,** 229(1992).
[6] H. Kleinert and S. V. Shabanov, Phys. Lett. A **232**, 327(1997).
[7] L. Kaplan, N. T. Maitra and E. J. Heller, Phys. Rev. A **56**, 2592(1997).
[8] J. R. Klauder, S. V. Shabanov, Nucl. Phys. B **511**, 713(1998).
[9] G. Ferrari and G. Cuoghi, Phys. Rev. Lett. **100**, 230403 (2008).
[10] B. Jensen and R. Dandoloff, Phys. Rev. A **80**, 052109 (2009).
[11] C. Ortix and J. van den Brink, Phys. Rev. B **81**, 165419 (2010); Phys. Rev. B **83**, 113406 (2011).
[12] Q. H. Liu, L. H. Tang, D. M. Xun, Phys. Rev. A **84,** 042101(2011).
[13] Q. H. Liu, arXiv:1109.0153v2, 4 Sept. 2011.
[14] M. V. Entin and L. I. Magarill, Phys. Rev. B **64**, 085330(2001). It is worthy of mentioning that one may wonder whether the momentum in the spin-orbit coupling electrons on a curved surface might be with the geometric momentum. It is not the case exactly. A proper treatment needs to start from the spin-orbit coupling term $\hbar/(4m^2)\mathbf{S}\cdot(\nabla V\times\mathbf{P})$ in three-dimensional flat space then confining it on the curved surface, where V is the crystal potential, $\mathbf{P}$ the electron momentum and $\mathbf{S}$ the spin operator, and the relation between the resultant expression and the geometric momentum is explored in depth.
[15] A.V. Chaplik and L. I. Magarill, Phys. Rev. Lett. **96**, 126402 (2006).
[16] M. P. López-Sancho and M. C. Muñoz, Phys. Rev. B **83**, 075406 (2011).
[17] Erhu Zhang, Shengli Zhang, and Qi Wang, Phys. Rev. B 75, 085308(2007).
[18] A. Szameit, et. al, Phys. Rev. Lett. **104**, 150403(2010).
[19] J. Onoe, T. Ito, H. Shima, H. Yoshioka and S. Kimura, Europhys. Lett. **98**, 27001(2012).
[20] Dirac's theory for a systems with second class constraints is not compatible with the Schrödinger's theory for the system. For instance, for quantum potential, Schrödinger's theory gives an unique result $V_g = -\hbar^2/(2\mu)(M^2 - K)$, whereas the Dirac's theory gives $V_g = -\hbar^2/(2\mu)(\alpha M^2 - \beta K)$ [5] with α and β two real parameters provided that Dirac bracket $\{f, g\}_D$ between two variables f and g in the theory is taken as the restriction of the symplectic form to the constraint surface in phase space. This compatibility problem is discussed in . However, I put forward a conjecture [12] that the arbitrariness with α and β can be fixed as $\alpha = \beta = 1$ once a correspondence of the equation of motion for the momentum $[p_i, H]/(i\hbar) \rightleftarrows \{p_i, H\}_D$ is imposed as a fundamental relation in the canonical quantization procedure.
[21] The terminology *geometric potential* was firstly introduced in A. V. Chaplik and R. H. Blick, New J. Phys. **6**, 33(2004), and the *embedding potential* was used in [26], the *curvature potential* in M. Encinosa and L. Mott, Phys. Rev. A **68**, 014102 (2003), the *quantum potential* in P. Maraner, Ann. Phys. **246**, 325 (1996) the *effective geometry-induced quantum potential*

in V. Atanasov, R. Dandoloff, A. Saxena, Phys. Rev. B **79**, 033404(2009), and the *curvature-induced effective potential* in H. Shima, H. Yoshioka, and J. Onoe, Phys. Rev. B **79**, 201401(R) (2009), etc. I think that *geometric potential and embedding potential are two appropriate names.*

[22] E. W Weisstein, "Intrinsic Curvature." From MathWorld–A Wolfram Web Resource. http://mathworld.wolfram.com/IntrinsicCurvature.html

[23] Q. H. Liu, C. L. Tong and M. M. Lai, J. Phys. A: Math. and Theor. **40**, 4161(2007).

[24] The geometric momentum $\mathbf{p}$ indeed describes purely a quantum motion on the surface for we can easily show $\mathbf{p}\cdot\mathbf{n}+\mathbf{n}\cdot\mathbf{p}=0$ with a relation $\nabla_2\cdot\mathbf{n}=-2H$ being used.

[25] C. E. Weatherburn, *Differential Geometry of Three Dimensions*, Vol. 1. (Cambridge University Press, 1930).

[26] S. Matsutani, J. Phys. A: Math. Gen. **26,** 5133(1993).

[27] M. Vos, I. McCarthy, Am. J. Phys. **65**, 544(1997), M. Vos, Aust. J. Phys. **51**, 609(1998).

[28] E. Weigold, I. McCarthy, *Electron Momentum Spectroscopy* (Kluwer Academic/Plenum, New York, 1999).

[29] Q. H. Liu, and T. G., Liu, Int. J. Theor. Phys. **42**, 2877(2003).

[30] X. M. Zhu, M. Xu, and Q. H. Liu, Int. J. Geom. Meth. Mod. Phys. **3**, 411(2010).

[31] For motions on a spherical surface, the initial constraint equation can be either $x^2+y^2+z^2=r^2$ or $x\dot{x}+y\dot{y}+z\dot{z}=0$ where $\dot{x}_i\equiv dx_i/dt$. The Dirac's theory for constrained systems can also give the geometric momentum. The calculations are available in references: T. Homma, T. Inamoto, T. Miyazaki, Phys. Rev. D **42**, 2049(1990), and T. Matsunaga, T. Miyazaki, M. Nojiri, C. Ohzeki and M. Yamanobe, Nuovo Cimento B, **113**, 975(1998). Unfortunately, in all these treatments, there are infinitely many sets of generalized momentum, each of them corresponds to a set of the local coordinates parameterizing the curved two-dimensional surface, including the geometric momentum. In order to single out the geometric momentum, a correspondence of the equation of motion for the momentum set $[p_i,H]/(i\hbar)\rightleftarrows\{p_i,H\}_D$ must be imposed, as proposed and discussed in Ref. [12].

[32] H. R. Sun, D. M. Xun, L. H. Tang, and Q. H. Liu, Commun. Theor. Phys. **58,** 31(2012).

[33] J. J. Sakurai, *Modern Quantum Mechanics*, Revised Edition (Addison-Wesley, New York. 2005).

[34] J. P. Dahl and M. Springborg, J. Chem. Phys. **88**, 4535 (1988).

[35] M. Ji, X. Gu, X. Li, X. G. Gong, J. Li, and L. S. Wang, Angew. Chem. Int. Ed. **44,** 7119-7123(2005).

[36] B. Coutant, and P. Brechignac, J. Chem. Phys. **91**, 1978-1986(1989).

[37] M. Vos, S. A. Canney, I. E. McCarthy, S. Utteridge, M. T. Michalewicz, and E. Weigold, Phys. Rev. B **56**, 1309-1315(1997).

[38] X. G. Ren, C. G. Ning, J. K. Deng, S. F. Zhang, G. L. Su, B. Li, and X. J. Chen, Chinese Phys. Lett. **22,** 1382(2005).

[39] M. Kjellberg, O. Johansson, F. Jonsson, A.V. Bulgakov, C. Bordas, E. E. B. Campbell, K. Hansen, Phys. Rev. A **81**, 023202(2010).

[40] B. C. Stipe, M. A. Rezaei and W. Ho, Science **279**, 1907(1998).

[41] J. Neumann, K. E. Gottschalk, and R. D. Astumian, ACS Nano. **6**, 5242-8(2012).

[42] N. Néel, L. Limot, J. Kröger, and R. Berndt, Phys. Rev. B. **77**, 125431(2008).

[43] J. Michl, and E. C. Sykes, ACS Nano. **3**, 1042(2009).